

CLAIMS

What is claimed is:

1. A method of modeling the effect of a molecular contaminant film on performance of an optical system, comprising the steps of:
 - correlating a mass of material outgassed from materials of the optical system to a spectrum of outgassed products;
 - normalizing the spectrum of outgassed products;
 - predicting an aggregate molecular contaminant film thickness from each material;
 - deriving an absorbance spectrum of the aggregate molecular contaminant film;
 - convolving the absorbance spectrum of the aggregate molecular contaminant film with an instrument function of the optical system; and
 - plotting at least one transmission band as a function of source temperature.
2. The method of claim 1, wherein the step of predicting the aggregate molecular film thickness includes the step of summing a weighted spectrum of each individual component's outgassed product to form the aggregate molecular contaminant film.
3. The method of claim 1, wherein the step of correlating the mass of material outgassed from materials of the optical system to a spectrum of outgassed products includes the steps of:
 - classifying each outgassed material into one of several groups based on at least one observed characteristic of the outgassed material;
 - obtaining an absorbance spectrum of a sample of the outgassed material; and
 - estimating a thickness of the sample of outgassed material based on the absorbance spectrum and the classification of the outgassed material.

4. The method of claim 3, wherein the step of obtaining the absorbance spectrum of the sample of the outgassed material includes the step of obtaining an average absorbance spectrum of a sample of the outgassed material.
5. The method of claim 3, wherein the step of classifying each outgassed material into one of several groups includes the groups consisting of a contaminant that is a pure substance that is a liquid at room temperature (Type 1 sample), a contaminant that is not a liquid or a pure substance but spectrum indicates that an absorbance in a region of interest is dominated by a single functional group (Type 2 sample), and a contaminant whose outgassing products are not a pure substance and cannot be represented by a single model compound that is a liquid (Type 3 sample).
6. The method of claim 5, further comprising the steps of:
 - estimating the thickness of the Type 1 sample based on the geometry of the Type 1 sample;
 - estimating the thickness of the Type 2 sample based on a known material that has a similar absorbance spectrum as the absorbance spectrum of the Type 2 sample; and
 - estimating the thickness of the Type 3 sample based on a synthetic spectrum constructed from model vectors of known materials that approximates the absorbance spectrum of the Type 3 sample.
7. The method of claim 6, wherein the step of estimating the thickness of the Type 1 sample includes the steps of:
 - estimating the thickness of the Type 1 sample based on a mass of the Type 1 sample, an area occupied by the Type 1 sample, and a density of the Type 1 sample.

8. The method of claim 6, wherein the step of estimating the thickness of the Type 2 sample includes the steps of:
 - selecting a material that has a similar absorbance spectrum as the absorbance spectrum of the Type 2 sample;
 - obtaining an absorbance spectrum of the selected material, wherein the thickness of the selected material is about 1 micron;
 - scaling the absorbance spectrum of the sample of the selected material by a scale factor to obtain a vector that approximates the strength of the absorbance spectrum of the Type 2 sample; and
 - estimating the thickness of the Type 2 sample as the product of the scale factor and the thickness of the selected material.
9. The method of claim 6, wherein the step of estimating the thickness of the Type 3 sample includes the steps of:
 - combining normalized vectors for known model compounds;
 - assigning a thickness to each vector;
 - manipulating the thickness assigned to each vector to construct an initial synthetic spectrum that approximates the absorbance spectrum of the Type 3 sample;
 - estimating the thickness of the Type 3 sample as the summation of the thickness assigned to each vector of the initial synthetic spectrum.
10. The method of claim 9, further comprising the steps of:
 - identifying an error region of the initial synthetic spectrum;
 - adding at least one normalized vector for known model compounds to the initial synthetic spectrum, wherein the at least one added vector compensates for a residue in the error region of the initial spectrum;
 - assigning a thickness to the at least one added vector;
 - manipulating the thickness of the at least one added vector to minimize the residue in the error region of the synthetic spectrum;
 - adding the manipulated thickness of the at least one vector to the estimated thickness of the Type 3 sample when the residue is positive; and

subtracting the manipulated thickness of the at least one vector to the estimated thickness of the Type 3 sample when the residue is negative.

11. The method of claim 9, further comprising the step of weighting the thickness of each model compound by the density of the compound.
12. The method of claim 3, further comprising the step of deriving a per unit absorbance spectrum of the sample of outgassed material.
13. A method of obtaining a per unit absorbance spectrum of a contaminant film when the thickness of the film is unknown, comprising the steps of:
 - collecting outgassed material from a compound;
 - classifying the outgassed material into one of several groups based on at least one observed characteristic of the outgassed material;
 - obtaining an absorbance spectrum of a sample of the outgassed material;
 - estimating a thickness of the sample of outgassed material based on the absorbance spectrum and the classification of the outgassed material;
 - and
 - scaling the absorbance spectrum of the sample of outgassed material by the estimated thickness of the sample of outgassed material.
14. The method of claim 13, wherein the step of obtaining the absorbance spectrum of the sample of the outgassed material includes the step of obtaining an average absorbance spectrum of a sample of the outgassed material.
15. The method of claim 13, wherein the step of classifying each outgassed material into one of several groups includes the groups consisting of a contaminant that is a pure substance that is a liquid at room temperature (Type 1 sample), a contaminant that is not a liquid or a pure substance but

spectrum indicates that an absorbance in a region of interest is dominated by a single functional group (Type 2 sample), and a contaminant whose outgassing products are not a pure substance and cannot be represented by a single model compound that is a liquid (Type 3 sample).

16. The method of claim 15, further comprising the steps of:
 - estimating the thickness of the Type 1 sample based on the geometry of the Type 1 sample;
 - estimating the thickness of the Type 2 sample based on a known material that has a similar absorbance spectrum as the absorbance spectrum of the Type 2 sample; and
 - estimating the thickness of the Type 3 sample based on a synthetic spectrum constructed from model vectors of known materials.
17. The method of claim 16, wherein the step of estimating the thickness of the Type 1 sample includes the steps of:
 - estimating the thickness of the Type 1 sample based on a mass of the Type 1 sample, an area occupied by the Type 1 sample, and a density of the Type 1 sample.
18. The method of claim 16, wherein the step of estimating the thickness of the Type 2 sample includes the steps of:
 - selecting a material that has a similar absorbance spectrum as the absorbance spectrum of the Type 2 sample;
 - obtaining an absorbance spectrum of the selected material, wherein the thickness of the selected material is about 1 micron;
 - scaling the absorbance spectrum of the sample of the selected material by a scale factor to obtain a vector that approximates the strength of the absorbance spectrum of the Type 2 sample; and
 - estimating the thickness of the Type 2 sample as the product of the scale factor and the thickness of the selected material.

19. The method of claim 16, wherein the step of estimating the thickness of the Type 3 sample includes the steps of:
- combining normalized vectors for known model compounds;
 - assigning a thickness to each vector;
 - manipulating the thickness assigned to each vector to construct an initial synthetic spectrum that approximates the absorbance spectrum of the Type 3 sample;
 - estimating the thickness of the Type 3 sample as the summation of the thickness assigned to each vector of the initial synthetic spectrum.
20. The method of claim 19, further comprising the steps of:
- identifying an overestimate region of the initial synthetic spectrum;
 - adding at least one normalized vector for known model compounds to the initial synthetic spectrum, wherein the at least one added vector compensates for overestimates made in the initial spectrum;
 - assigning a thickness to the at least one added vector;
 - manipulating the thickness of the at least one added vector to reduce a residue of the synthetic spectrum;
 - adding the manipulated thickness of the at least one vector to the estimated thickness of the Type 3 sample when the residue is positive; and
 - subtracting the manipulated thickness of the at least one vector to the estimated thickness of the Type 3 sample when the residue is negative.
21. The method of claim 19, further comprising the step of weighting the thickness of each model compound by the density of the compound.
22. A computer system for modeling the effect of a molecular contaminant film on performance of an optical system, comprising:
- a storage medium;
 - at least one processor, wherein the processor is operatively coupled to the storage medium;

a computer program residing on the storage medium and executed by the at least one processor, wherein the computer program causes the processor to

correlate a mass of material outgassed from materials of the optical system to spectrum of outgassed products;

normalize the spectrum of outgassed products;

predict an aggregate molecular contaminant film thickness from each material;

convolve an absorbance spectrum of the aggregate molecular contaminant film with an optical system instrument function; and

plot at least one transmission band as a function of source temperature.

23. The system of claim 22, wherein a weighted spectrum of each individual component's outgassed product is summed to predict the aggregate molecular contaminant film thickness.

24 The system of claim 22, wherein the computer program further causes the processor to:

classify each outgassed material into one of several groups based on at least one observed characteristic of the outgassed material;

obtain an absorbance spectrum of a sample of the outgassed material; and

estimate a thickness of the sample of outgassed material based on the absorbance spectrum and the classification of the outgassed material.

25. The system of claim 24, wherein the computer program further causes the processor to:

obtain an average absorbance spectrum of a sample of the outgassed material.

26. The system of claim 24, wherein the computer program further causes the processor to:

classify each outgassed material into the groups consisting of a contaminant that is a pure substance that is a liquid at room temperature (Type 1 sample), a contaminant that is not a liquid or a pure substance but spectrum indicates that an absorbance in a region of interest is dominated by a single functional group (Type 2 sample), and a contaminant whose outgassing products are not a pure substance and cannot be represented by a single model compound that is a liquid (Type 3 sample).

27. The system of claim 26, wherein the computer program further causes the processor to:

estimate the thickness of the Type 1 sample based on the geometry of the Type 1 sample;

estimate the thickness of the Type 2 sample based on a known material that has a similar absorbance spectrum as the absorbance spectrum of the Type 2 sample; and

estimate the thickness of the Type 3 sample based on a synthetic spectrum constructed from model vectors of known materials that approximates the absorbance spectrum of the Type 3 sample.

28. The system of claim 27, wherein the computer program further causes the processor to:

estimate the thickness of the Type 1 sample based on a mass of the Type 1 sample, an area occupied by the Type 1 sample, and a density of the Type 1 sample.

29. The system of claim 27, wherein the computer program further causes the processor to:

select a material that has a similar absorbance spectrum as the absorbance spectrum of the Type 2 sample;

obtain an absorbance spectrum of the selected material, wherein the thickness of the selected material is about 1 micron;

scale the absorbance spectrum of the sample of the selected material by a scale factor to obtain a vector that approximates the strength of the absorbance spectrum of the Type 2 sample; and

estimate the thickness of the Type 2 sample as the product of the scale factor and the thickness of the selected material.

30. The system of claim 27, wherein the computer program further causes the processor to:

combine normalized vectors for known model compounds;

assign a thickness to each vector;

manipulate the thickness assigned to each vector to construct an initial synthetic spectrum that approximates the absorbance spectrum of the Type 3 sample;

estimate the thickness of the Type 3 sample as the summation of the thickness assigned to each vector of the initial synthetic spectrum.

31. The system of claim 30, wherein the computer program further causes the processor to:

identify an error region of the initial synthetic spectrum;

add at least one normalized vector for known model compounds to the initial synthetic spectrum, wherein the at least one added vector compensates for a residue in the error region of the initial spectrum;

assign a thickness to the at least one added vector;

manipulate the thickness of the at least one added vector to minimize the residue in the error region of the synthetic spectrum;

add the manipulated thickness of the at least one vector to the estimated thickness of the Type 3 sample when the residue is positive; and

subtract the manipulated thickness of the at least one vector to the estimated thickness of the Type 3 sample when the residue is negative.

Docket No. PD-03W041

32. The system of claim 29 wherein the computer program further causes the processor to weight the thickness of each model compound by the density of the compound.
33. The method of claim 24, wherein the computer program further causes the processor to derive a per unit absorbance spectrum of the sample of outgassed material.
34. The method of claim 22, wherein the computer program further causes the processor to generate a contour plot, wherein the contour plot includes the at least one transmission band plotted as a function of a source temperature for a range of aggregate molecular contaminant film thicknesses.
35. The method of claim 22, wherein the computer program further causes the processor to:
- calculate a ratio of a first transmission band and a second transmission band; and
 - plot the ratio as a function of a source temperature.
36. The method of claim 1, wherein the step of correlating the mass of material outgassed from materials of the optical system to the spectrum of outgassed products includes using an infrared spectrum of outgassed products.
37. The method of claim 1, wherein the step of correlating the mass of material outgassed from materials of the optical system to the spectrum of outgassed products includes using a mass of material outgassed from organic materials.